CHEMISTRY OF THE COPPER-SILICON INTERFACE

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Copper and silicon readily interdiffuse, even at room temperature, to form an interface which can be several nanometers thick [1]. Over the years considerable effort has gone into investigating this diffusion process and chemical nature of the interface that forms. Photoemission measurements give evidence for the formation of a stable silicide with a definite stoichiometry, Cu_3Si [2]. This is evidenced by the splitting of the Si LVV Auger line [3] and a slight shift and change in shape of the copper valence band density of states (DOS) as measured by ultra-violet-photoemission [4]. Other studies suggest that an alloy forms with average stoichiometry close to Cu_3Si [5].

Electron Momentum Spectroscopy (EMS) directly maps the probability density of the target electrons in energy-momentum space producing measurements of the full band structure (dispersion and electron density) of the solid. This enables a detailed investigation of the copper-silicon interface to be performed. Details of the spectrometer used can be found elsewhere [6]. Briefly, incident electrons with an energy of about 20 keV are used to eject a bound target electron, with the simultaneous detection of both outgoing electrons. The energy and momentum of the outgoing electrons are accurately measured, therefore, conservation laws can be used to determine the binding energy and momentum of the target electron at the instant of ionisation. For this study the binding energy and momentum range of interest was 0-20 eV and 0-1.5 a.u. respectively, with a resolution of ~ 1 eV and 0.1 a.u. respectively.

Density Functional Theory calculations have been performed for Cu_7Si_3, bulk silicon and bulk copper, specifically using the local density approximation Hamiltonian, with Dirac-Slater exchange [7] and Vosko-Wilk-Nusair correlation [8].

We present experimental and calculated band structures and DOS for copper-silicide, Cu and Si. Calculated DOS of Cu and copper-silicide are dominated by the Cu 3d bands, and differences between the two solids is relatively small. Photoemission is dominated by the 3d bands. By contrast, the calculated full valence band structures for the two solids are quite distinct. EMS measures this band structure and thus is able reveal the chemistry of the copper silicon interface, and determine the nature of the copper-silicon interaction within the interface.

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